# 2,4-DIMETHYLDIPHENYLSULPHONE

**Other names:** Sulfone, phenyl, 2,4-xylyl
**Inchi:** InChI=1S/C14H14O2S/c1-11-8-9-14(12(2)10-11)17(15,16)13-6-4-3-5-7-13/h3-10H,1-2H3
**InchiKey:** ZCVSDPUSEUOUHQ-UHFFFAOYSA-N
**Formula:** C14H14O2S
**SMILES:** Cc1ccc(S(=O)(=O)c2ccccc2)c(C)c1
**Mol. weight [g/mol]:** 246.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -172.03 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 30.70 | kJ/mol | Joback Method |
| ie | 8.55 | eV | Cheméo Relay (1.0) |
| log10ws | -4.38 | | Cheméo Relay (1.0) |
| logp | 3.136 | | Crippen Method |
| mcvol | 188.690 | ml/mol | McGowan Method |
| tb | 641.75 | K | Cheméo Relay (1.0) |
| tf | 358.00 ± 2.00 | K | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 456.66 | J/mol×K | 630.82 | Joback Method |
| cpg | 473.14 | J/mol×K | 669.29 | Joback Method |
| cpg | 488.39 | J/mol×K | 707.76 | Joback Method |
| cpg | 502.46 | J/mol×K | 746.22 | Joback Method |
| cpg | 515.36 | J/mol×K | 784.69 | Joback Method |
| cpg | 527.14 | J/mol×K | 823.16 | Joback Method |
| cpg | 537.83 | J/mol×K | 861.63 | Joback Method |

## Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4212742&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |